One-Dimensional Disordered Systems and Scattering Theory

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Methods from scattering theory are applied to one dimensional disordered systems. This approach (i) gives a relation between the scattering phase shift and the integrated density of states, (ii) provides a very natural connection with random matrix theory and allows to study the special energies, where the transmission probability does not vanish in the infinite length limit.

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One-dimensional disordered quantum systems in one-particle approximation play an important role in a number of different physical contexts. Examples include mesoscopic conductors like quantum, atomic and molecular wires [1]. Applications of scattering theory to these systems have a long history and are now of renewed interest due to advances in technology that allow the construction of devices at nanometric scales. Already in the late fifties it was recognized that the electric dc conductivity in such quasi-one-dimensional structures is directly related to scattering probabilities [2]. From the viewpoint of the Kubo formula this relation is discussed in Refs. [3,4]. For systems of finite size the connection between the density of states (DOS) and the scattering phase is considered in [5]. Also scattering theory naturally arises in the study of the localization of the electromagnetic waves in dielectric multilayers [6].

In this letter we report on some rigorous results when applying scattering theory to the one-dimensional Schrödinger equation $-\psi'' + V_{lm}(x)\psi = E\psi$ with a potential $V_{lm}(x) = \sum_{j=-l}^{m} \alpha_j f(x-j)$ in the limit of large number of scatterers $n = l+m+1 \to \infty$. In particular we address the question how the Lyapunov exponent (LE) and DOS can be reconstructed in terms of the S-matrices of the single-site Hamiltonians $H_\alpha = H_0 + \alpha f$. This approach exhibits a very natural connection with the random matrix theory. A part of the results presented here will appear in more complete form with proofs elsewhere [7]. For other applications of scattering theory to Schrödinger operators with periodic and random potentials we refer to [8,9] and [10], respectively.

The single-site potential $f \geq 0$ is supposed to be a piecewise continuous bounded function on the interval $[-1/2, 1/2]$, and α_j is a sequence of uniformly bounded reals (random or as a special case deterministic), $|\alpha_j| \leq \alpha$. In the random case α_j is a metrically transitive sequence of i.i.d. (independent, identically distributed) variables having a common distribution (measure) ν, which has support in a finite interval $[\alpha_-, \alpha_+]$. Let $H^{(lm)} = H_0 + V_{lm}$ be the Hamiltonian involving n sites and let $H_j = H_0 + \alpha_j f(\cdot - j)$ be the single-site Hamiltonian. By $S^{(lm)}(E)$ and $S_j(E)$ we denote the corresponding S-matrices,

$$S^{(lm)}(E) = \begin{pmatrix} T^{(lm)}(E) & R^{(lm)}(E) \\ L^{(lm)}(E) & T^{(lm)}(E) \end{pmatrix}, \qquad S_j(E) = \begin{pmatrix} T_j(E) & R_j(E) \\ L_j(E) & T_j(E) \end{pmatrix}, \tag{1}$$

with T being the transmission amplitudes and R and L the right and left reflection amplitudes respectively. We also consider the matrices

$$\Lambda^{(lm)}(E) = \begin{pmatrix} \frac{1}{T^{(lm)}(E)} & -\frac{R^{(lm)}(E)}{T^{(lm)}(E)} \\ \frac{L^{(lm)}(E)}{T^{(lm)}(E)} & \frac{1}{T^{(lm)}(E)^*} \end{pmatrix}, \qquad \Lambda_j(E) = \begin{pmatrix} \frac{1}{T_j(E)} & -\frac{R_j(E)}{T_j(E)} \\ \frac{L_j(E)}{T_j(E)} & \frac{1}{T_j(E)^*} \end{pmatrix}.$$

From the unitarity of the scattering matrix it follows that the matrices $\Lambda^{(lm)}(E)$ and $\Lambda_j(E)$ are unimodular.

The scattering phase $\delta^{(lm)}(E)$ for $H^{(lm)}$ is related to its S-matrix by $\delta^{(lm)}(E) = \ln\det S^{(lm)}(E)/2i$ and $T^{(lm)}(E) = |T^{(lm)}(E)|e^{i\delta^{(lm)}(E)}$. Both the scattering phase and the distribution of the bound states can be described in terms of the Lifshitz-Krein spectral shift function (SSF) [11] $\xi^{(lm)}(E)$. In fact, $\xi^{(lm)}(E) = -\pi\delta^{(lm)}(E)$ for $E > 0$ and equals minus the number of bound states below $E < 0$. This is the well-known Birman-Krein theorem [11]. It is the general version of the well-known result of Beth and Uhlenbeck [12], which relates scattering data to the second virial coefficient.

It is natural to expect that $\xi^{(lm)}(E)/n$ is a self-averaging quantity. Indeed we show [7] that $\widetilde{\xi}^{(lm)}_{\pm}(E) = \xi^{(lm)}(E) \pm 1$ is sub/super-additive with respect to the interval length $(-l, m)$, and therefore by the Akcoglu-Krengel ergodic theorem [13]

$$\lim_{l,m\to\infty} \xi^{(lm)}(E)/n =: \xi(E) \tag{2}$$

exists almost surely and is non-random. We call this limit the spectral shift density (SSD). For all $E > 0$ it satisfies the inequality $\langle\xi_{\underline{\alpha}}(E)\rangle - 1/2 \le \xi(E) \le \langle\xi_{\underline{\alpha}}(E)\rangle + 1/2$. Here $\langle\xi_{\underline{\alpha}}(E)\rangle$ denotes the site average $\lim_{n\to\infty}\sum_{j=-l}^{j=m}\xi_{\alpha_j}(E)/n$ with $\xi_{\alpha_j}(E)$ being the SSF for H_{α_j}. Similar inequalities holds for $E \le 0$ with 1 instead of $1/2$. Moreover, $\xi(E) \ge 0$ (≤ 0) if all α_j's are positive (negative). Also $\xi(E) = N_0(E) - N(E)$, the difference of the integrated densities of states for the free and the interacting cases. Recalling that $d\delta^{(n)}(E)/dE$ is the time-delay during the scattering process [14], we can interpret $-\xi(E)/\pi$ as the integrated time-delay density, such that $-\xi'(E)/\pi$ is the time-delay per unit length.

A result similar to (2) is known [4,16] to hold for the transmission coefficient,

$$\lim_{l,m\to\infty} \ln|T^{(lm)}(E)|/n = -\gamma(E), \tag{3}$$

which is minus the LE, i.e. the inverse localization length, at energy $E > 0$. It satisfies the inequality $\gamma(E) \le -\langle\ln|T_{\underline{\alpha}}(E)|\rangle + \ln 2$, where $\langle\ln|T_{\underline{\alpha}}(E)|\rangle = \lim_{l,m\to\infty}\sum_{j=-l}^{j=m}\ln|T_{\alpha_j}|/n$. In particular, the positiveness of the Lyapunov exponent implies the absence of an absolutely continuous spectrum [17]. Perturbation of the periodic potential by a finite number of impurities does not change $\gamma(E)$ and $\xi(E)$. The LE is positive within the gaps of the spectrum and equals zero within the bands. For E being the impurity level in a gap of the continuous spectrum $\gamma(E)$ is the inverse localization length of the impurity wave functions $|\psi(x)| \sim Ce^{-\gamma(E)|x|}$ (for a special case this was proven in [15]).

Since for positive energies $\gamma_0(E) = 0$ (the LE for the free Hamiltonian H_0), we can combine (2) and (3) in the form

$$\lim_{l,m\to\infty} \ln T^{(lm)}(E)/n = -\gamma(E) - i\pi\xi(E) = w(E) - w_0(E),$$

where $w(E) = -\gamma(E) + i\pi N(E)$ and $w_0(E) = -\gamma_0 + i\pi N_0(E)$. Actually $w(E)$ and $w_0(E)$ can be analytically continued into the complex energy half-plane such that e.g. $w_0(E) = -\lim_{\epsilon\to 0}\sqrt{-E + i\epsilon}$. In the periodic case $w(z)$ is related to the quasimomentum $k(z) = -iw(z)$.

Now we employ the Aktosun factorization formula [18], which states

$$\Lambda^{(lm)}(E) = \prod_{j=-l}^{m} \Lambda_j(E), \tag{4}$$

where the product is understood in the ordered sense, i.e. $\Lambda_{-l}\ldots\Lambda_m$. From (2) and (3) it follows that

$$\gamma(E) \pm i\pi\xi(E) = \lim_{l,m\to\infty} \ln(e_\pm, \Lambda^{(lm)}(E)e_\pm)/n$$

almost surely with $e_+ = (1,0)^T$, $e_- = (0,1)^T$ and $(\cdot,\cdot)$ being the inner product in $\mathbb{C}^2$. In analogy to (1) we denote by $T_\alpha(E)$, $R_\alpha(E)$, and $L_\alpha(E)$ the elements of the scattering matrix at energy $E > 0$ for H_α. With

$$U_E = \begin{pmatrix} e^{-i\sqrt{E}} & 0 \\ 0 & e^{i\sqrt{E}} \end{pmatrix}, \qquad \Lambda_\alpha(E) = \begin{pmatrix} \frac{1}{T_\alpha(E)} & -\frac{R_\alpha(E)}{T_\alpha(E)} \\ \frac{L_\alpha(E)}{T_\alpha(E)} & \frac{1}{T_\alpha(E)^*} \end{pmatrix}$$

it follows from the Aktosun factorization formula (4) that

$$\Lambda^{(lm)}(E) = \prod_{j=-l}^{m} U_E^j \Lambda_{\alpha_j}(E) U_E^{-j} = U_E^{-l-1/2} \cdot \prod_{j=-l}^{m} U_E^{1/2} \Lambda_{\alpha_j}(E) U_E^{1/2} \cdot U_E^{-m-1/2}. \tag{5}$$

Since $U_E e_\pm = \exp\{\pm i\sqrt{E}\} e_\pm$ one obtains that the r.h.s. of (5) equals

$$e^{\pm i\sqrt{E}n}\left(e_\pm, \prod_{j=-l}^{m} \widetilde{\Lambda}_{\alpha_j}(E) e_\pm\right), \qquad \widetilde{\Lambda}_\alpha(E) = U_E^{1/2}\Lambda_\alpha(E) U_E^{1/2} = \begin{pmatrix} \frac{e^{i\sqrt{E}}}{T_\alpha(E)} & -\frac{R_\alpha(E)}{T_\alpha(E)} \\ \frac{L_\alpha(E)}{T_\alpha(E)} & \frac{e^{-i\sqrt{E}}}{T_\alpha(E)^*} \end{pmatrix}.$$

From $\xi(E) = N_0(E) - N(E) = \sqrt{E}/\pi - N(E)$ it follows that

$$\gamma(E) \mp i\pi N(E) = \lim_{n\to\infty} \frac{1}{n} \ln\left(e_\pm, \prod_{j=-l}^{m} \widetilde{\Lambda}_{\alpha_j}(E) e_\pm\right). \tag{6}$$

The phase of the logarithm is unambigously fixed by the recurrence inequalities $|\xi^{(l,m+1)} - \xi^{(lm)} - \xi_{\alpha_{m+1}}| \leq 1/2$ and $|\xi^{(l+1,m)} - \xi^{(lm)} - \xi_{\alpha_{l+1}}| \leq 1/2$. If the α_j's form a sequence of random i.i.d. variables, for every $E > 0$ the sequence $\widetilde{\Lambda}_{\alpha_j}(E)$ is a sequence of random i.i.d. unimodular matrices.

Eq. (6) establishes a connection between the spectral theory of one-dimensional disordered systems on the one hand and scattering theory and the theory of random matrices on the other hand. We outline some of its applications. In the periodic case $\alpha_j = \alpha$ Hill's discriminant [19] is related to the scattering characteristics of H_α [8] by $\Delta_\alpha(E) = 2\cos(\sqrt{E} - \pi\xi_\alpha(E))/|T_\alpha(E)|$. From (6) it follows that

$$\gamma(E) = \begin{cases} \log\left[\frac{1}{2}\left(|\Delta_\alpha(E)| + \sqrt{\Delta_\alpha(E)^2 - 4}\right)\right], & |\Delta_\alpha(E)| > 2 \\ 0, & |\Delta_\alpha(E)| \leq 2 \end{cases}$$

and $\cos(\pi N(E)) = \Delta_\alpha(E)/2 - \cosh\gamma(E)$. The approximate LE and the SSD according to (6) for $n = 7,\ 15$ and single-site δ-potentials (finite Kronig-Penney model) are presented in Fig. 1. It shows that the infinite limit is already well approximated by the finite system with only few sites. In particular the appearance of the band structure is already clearly visible.

In the random case $\gamma(E) > 0$ almost everywhere since the absolutely continuous spectrum is empty [17]. Employing the random matrix theory we completely characterize the set S of those energies, where the LE vanishes. If the distribution ν of α_j's has an absolutely continuous component, S is the union of S_0 and $S_\pm$, where S_0 is the set of those E's for which $R_\alpha(E) = 0$ for all α. The sets $S_\pm$ are subsets of $\{(\pi k)^2,\ k \in \mathbb{N}\}$ for which the functions

$$F_E^{(\pm)}(\alpha) = \left(-i\sin(\sqrt{E} - \pi\xi_\alpha(E)) \pm \sqrt{\cos^2(\sqrt{E} - \pi\xi_\alpha) - |T_\alpha(E)|^2}\right) / R_\alpha(E) e^{i\pi\xi_\alpha(E)}$$

do not depend on α [7]. The case when ν is a discrete measure can be considered similarly. In particular, when f is the square barrier of unit length and height, and α_j's take only two values 0 and β with probability 1/2, one gets that S consists of those $E > 0$ which can be represented either as $(\pi k)^2$ or as $\beta + (\pi k)^2$ with an integer k (Fig. 2). We numerate them in increasing order and denote them by E_j and $\widehat{E}_j$ respectively. For these values of the energy E the transmission probability $|T^{(lm)}(E)|^2$ does not vanish as $l, m \to \infty$ for all possible configurations α_j in contrast to the Azbel resonances [20]. We found that $|T^{(lm)}(\widehat{E}_j)|^2 = 1$ for all l, m and j, whereas $|T^{(lm)}(E_j)|^2$ are not self-averaging quantities and strongly fluctuate with the variation of the number of sites n remaining, however, sufficiently far from zero (Fig. 3). The existence of energies with non-vanishing transmittivity can lead to a significant enhancement of the conductivity in real quasi-one-dimensional disordered systems. Earlier the "reflectionless" energies were found for the tight-binding model with off-diagonal disorder [21]. It is worth to emphasize that in the general case (i.e. for arbitrary f and ν) $\gamma(E) = 0$ for some E does not imply directly that $T^{(l,m)}(E)$ remains nonzero for all l and m. For example, $\gamma(E) = 0$ if $T^{(l,m)}(E)$ tends to zero slower then exponentially with $n \to \infty$.

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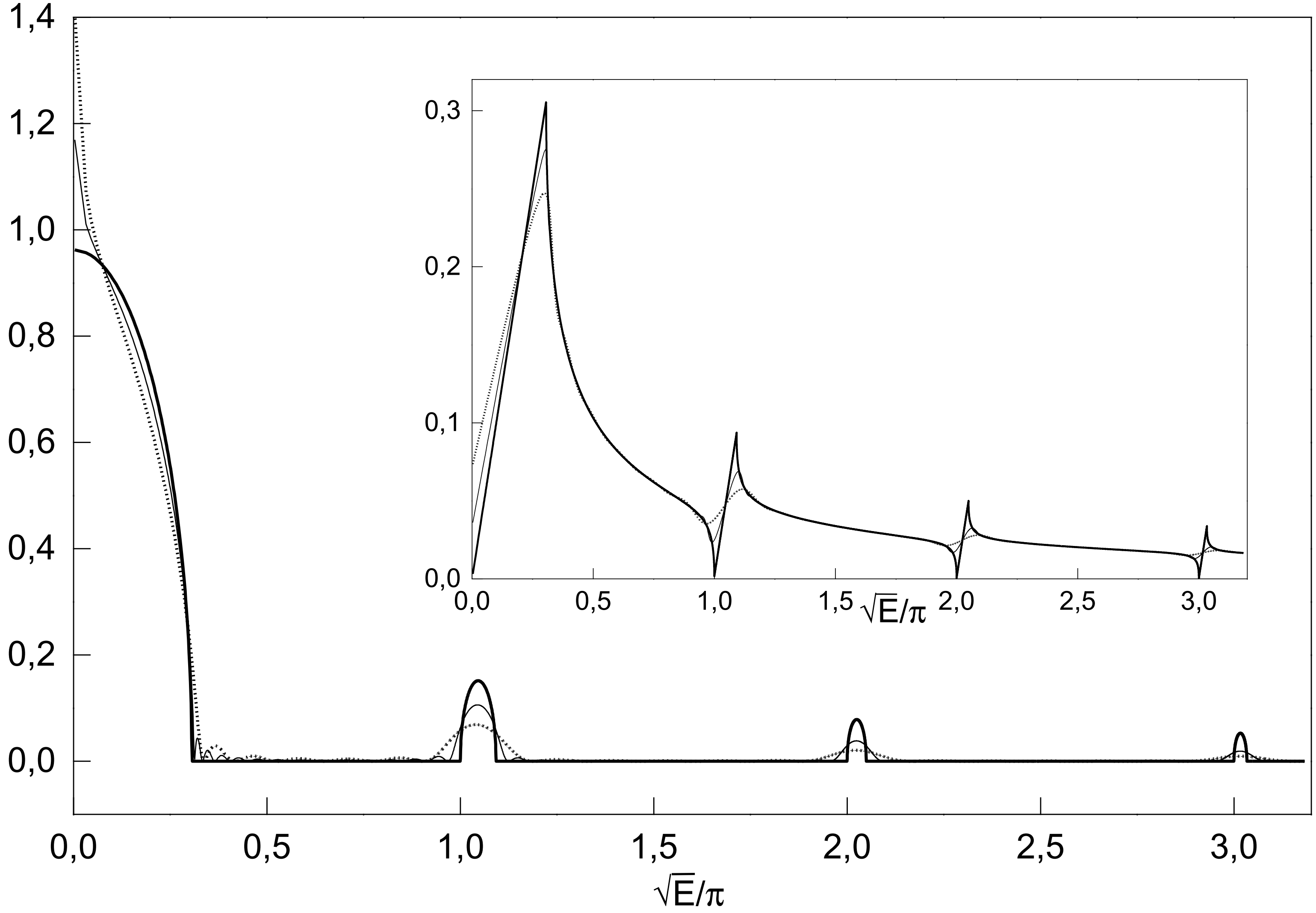
Fig. 1: The Lyapunov exponent and the spectral shift density (inset) for the deterministic Kronig-Penney model with $\alpha = 1$ (thick solid lines). The dotted and thin solid lines represent $-\ln|T^{(lm)}(E)|/n$ and $\xi^{(lm)}(E)/n$ for $n = 7$ and for $n = 15$ respectively.

Fig. 2: The Lyapunov exponent and the spectral shift function (inset) for the binary random model with $\beta = -60$ and f being the unit step potential. The arrows mark the points where $\gamma(E)$ vanishes.

Fig. 3: Fluctuations of the transmission probability $|T^{(lm)}(E_2)|^2$ vs number of sites n for the binary random modell as in Fig. 2.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2,0
2,5
3,0
$\sqrt{E}/\pi$
0,3
0,2
0,1
0,0
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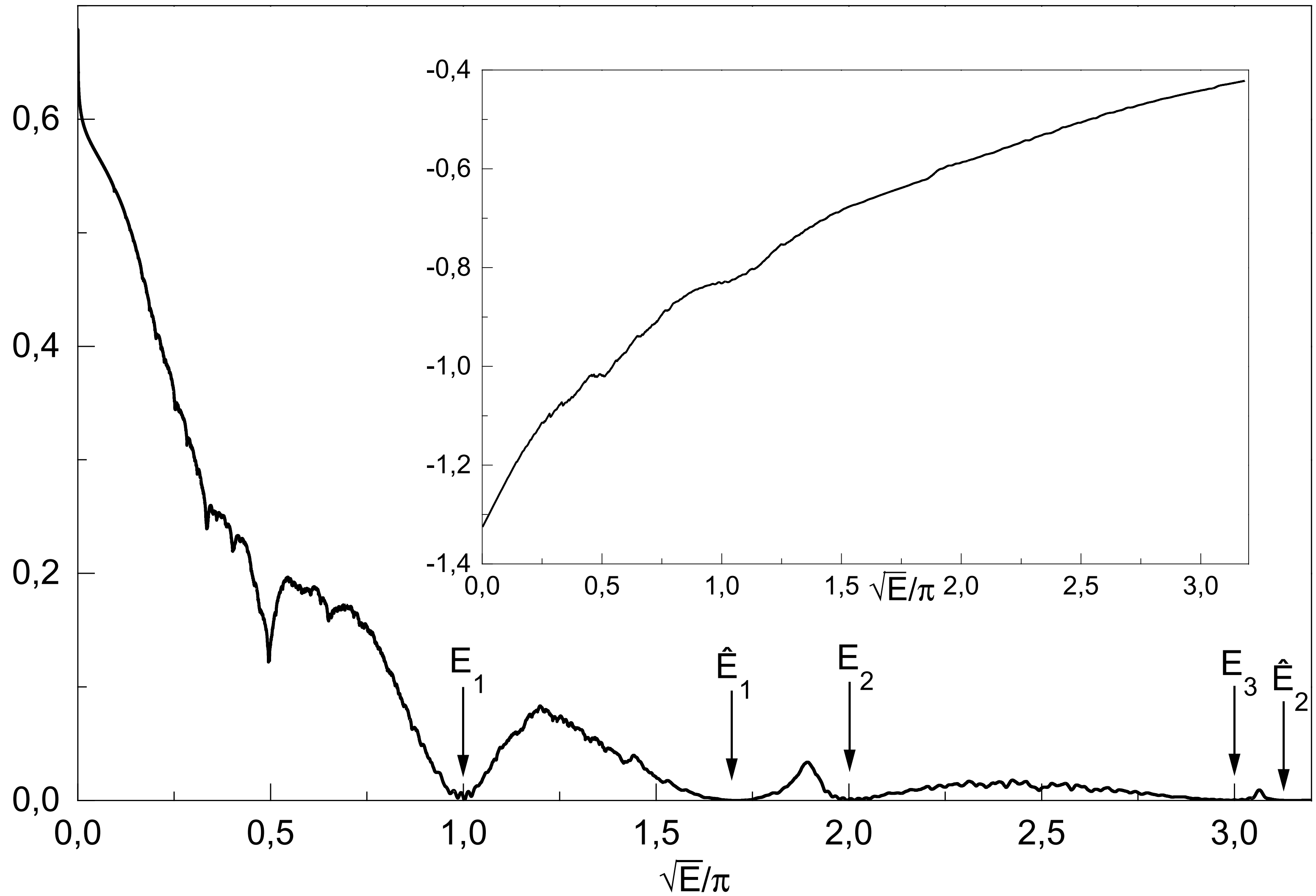
0,5
1,0
1,5
$\sqrt{E}/\pi$
2,0
2,5
3,0

FIG. 1.

FIG. 2.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E_1
$\hat{E}_1$
E_2
E_3
$\hat{E}_2$
-0,4
-0,6
-0,8
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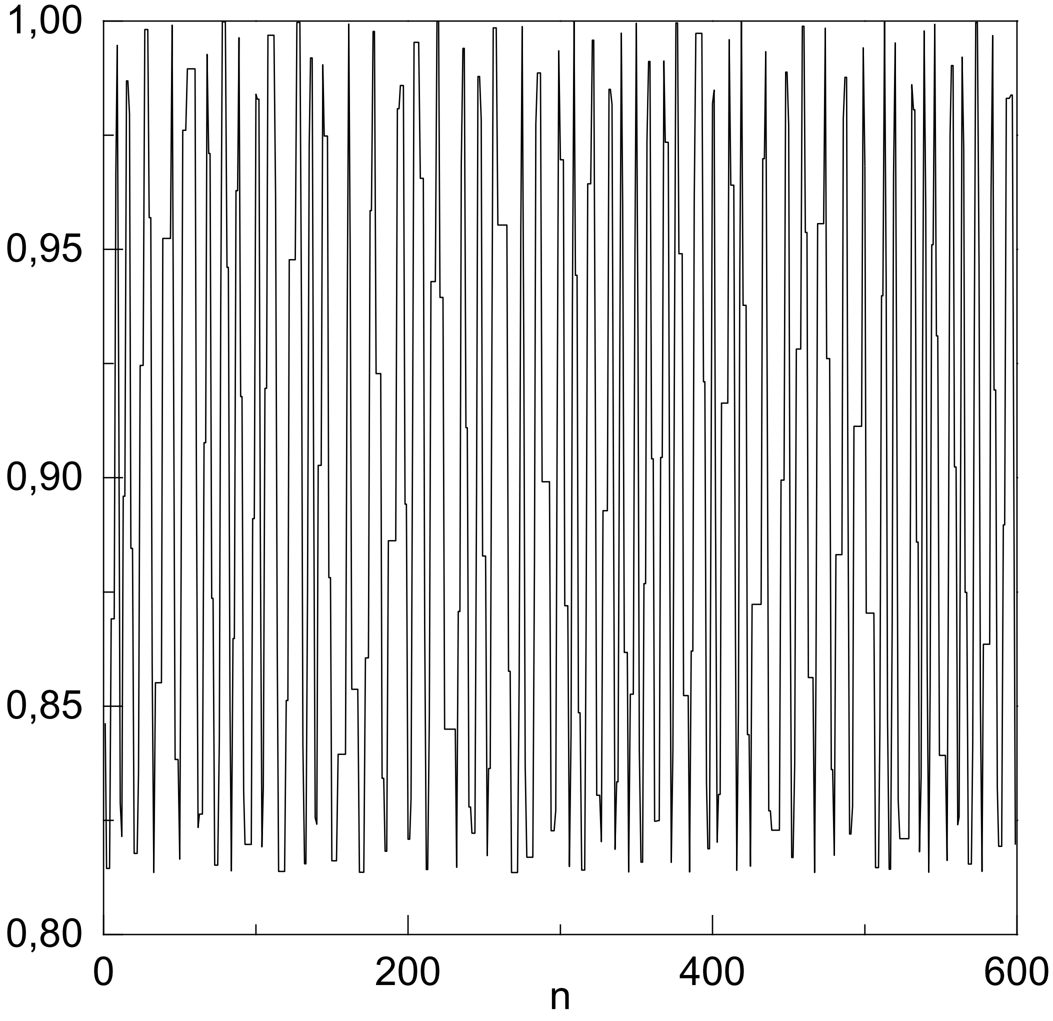

FIG. 3.